Reducing the Theoretical Uncertainty in Extracting $|V_{ub}|$ from the Inclusive $B \to X_u \ell^- \overline{\nu}_\ell$ Decay Rate

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Abstract. Utilizing asymptotic Padé-approximant methods, we estimate the three-loop order $\overline{MS}$ coefficients of $\alpha_s^3 [\log(\mu^2/m_b^2(\mu))]^k$ terms [$k = \{0,1,2,3\}$] within the $b \to u \ell^- \overline{\nu}_\ell$ decay rate. Except for the coefficient of the $k = 0$ term, all other coefficients may also be obtained via renormalization-group (RG) methods. The relative errors in asymptotic Padé-approximant estimates of the $k = \{1,2,3\}$ terms are found to be 5.1% or less, thereby providing an estimate of the theoretical uncertainty in the asymptotic Padé-approximant estimate of the RG-inaccessible $k = 0$ term. By a judicious choice in the renormalization scale parameter, we are able to extract $|V_{ub}|$ from the inclusive decay rate to within $\pm 7\%$ theoretical uncertainty.

INTRODUCTION

The inclusive semileptonic $B \to X_u \ell^- \overline{\nu}_\ell$ decay rate is sensitive only to a single mass parameter, the b-quark mass m_b, since the u-quark, charged lepton, and associated antineutrino are all very light compared to m_b. This property makes the calculated decay rate particularly attractive for the extraction of the CKM mixing parameter $|V_{ub}|$. QCD corrections to the rate have recently been calculated to two-loop order within an $\overline{MS}$ scheme [1]. If the renormalization scale μ is chosen to be $m_b(m_b) \cong 4.2\,GeV$ [2], i.e., if $\mu = m_b(\mu)$, then the two loop rate is given by

$$\Gamma(B \to X_u \ell^- \overline{\nu}_\ell) = K m_b^5(m_b) \left[1 + 0.30 + 0.14\right], \ \ K \equiv G_F^2 |V_{ub}|^2/192\pi^3. \quad (1)$$

Determinations of $|V_{ub}|$ based upon comparison of experimental results to this expression are necessarily subject to theoretical uncertainties associated with the premature truncation of the slowly convergent perturbative series in (1). In the present work, we demonstrate how asymptotic Padé-approximant methods in conjunction with renormalization-group (RG-) methods can dramatically reduce such theoretical uncertainties . . .

1) by providing an estimate of three loop contributions to the decay rate that can be tested against RG-accessible three-loop coefficients in the rate, and

2) by demonstrating that the physically-motivated choice of scale parameter μ which minimizes scale sensitivity [3] is quite close to that which minimizes the size of the four-loop term, and consequently, the truncation error for an asymptotic series.

DETERMINATION OF RG-ACCESSIBLE THREE-LOOP COEFFICIENTS

The series portion $S[x, L]$ of the perturbative $\overline{MS}$ expression for the inclusive semileptonic rate,

$$\Gamma\left(B \to X_u \ell^- \overline{\nu}_\ell\right) = K \left[m_b^{(n_f)}(\mu)\right]^5 S\left[x(\mu), L(\mu)\right], \tag{2}$$

may be expressed in terms of the QCD expansion parameter

$$x(\mu) \equiv \alpha_s^{(n_f)}(\mu)/\pi \tag{3}$$

and n^{th}-order polynomials of logarithms

$$L(\mu) \equiv \log\left(\left[\mu/m_b^{(n_f)}(\mu)\right]^2\right) \tag{4}$$

appearing within the series coefficient of $x^n(\mu)$. The superscript n_f indicates the number of active flavours contributing to the evolution of the QCD coupling constant α_s and the running b-quark mass. Thus, the series $S[x, L]$ within (2) is of the form

$$\begin{aligned} S[x, L] &= 1 + x\left(a_0 + a_1 L\right) + x^2\left(b_0 + b_1 L + b_2 L^2\right) \\ &+ x^3\left(c_0 + c_1 L + c_2 L^2 + c_3 L^3\right) + \mathcal{O}\left(x^4\right). \end{aligned} \tag{5}$$

The one- and two-loop coefficients a_0, a_1, b_0, b_1, and b_2 have been calculated for arbitrary n_f in [1]. For example, if $n_f = 5$,

$$a_0 = 4.25360, \ a_1 = 5, \ b_0 = 26.7848, \ b_1 = 36.9902, \ b_2 = 17.2917. \tag{6}$$

Note that the parameter μ within (3) and (4) is the (nonphysical) renormalization scale parameter. The full decay rate (2) must ultimately be independent of the choice of μ:

$$0 = \frac{1}{K m_b^5}\left(\mu^2 \frac{d\Gamma}{d\mu^2}\right) = \left[(1 - 2\gamma(x))\frac{\partial}{\partial L} + \beta(x)\frac{\partial}{\partial x} + 5\gamma(x)\right] S[x, L], \tag{7}$$

$$\beta(x) = -\left(\beta_0 x^2 + \beta_1 x^3 + \beta_2 x^4 + \ldots\right), \tag{8}$$

$$\gamma(x) = - \left(\gamma_0 x + \gamma_1 x^2 + \gamma_2 x^3 + \ldots \right), \tag{9}$$

where, for $n_f = 5$, $\beta_0 = 23/12$, $\beta_1 = 29/12$, $\beta_2 = 9769/3456$, $\gamma_0 = 1$, $\gamma_1 = 253/72$, and $\gamma_2 = 7.4195$ [2]. If we expand the final line of (7) perturbatively in powers of $x^k L^m$, we find that

$$0 = x \left(a_1 - 5\gamma_0 \right) + x^2 \left(b_1 - a_0\beta_0 - 5a_0\gamma_0 + 2a_1\gamma_0 - 5\gamma_1 \right) + x^2 L \left(2b_2 - a_0\beta_0 - 5a_1\gamma_0 \right)$$

$$+ x^3 \left(c_1 - 2b_0\beta_0 - a_0\beta_1 - 5b_0\gamma_0 + 2b_1\gamma_0 - 5a_0\gamma_1 + 2a_1\gamma_1 - 5\gamma_2 \right)$$

$$+ x^3 L \left(2c_2 - 2b_1\beta_0 - a_1\beta_1 - 5a_1\gamma_1 - 5b_1\gamma_0 + 4b_2\gamma_0 \right)$$

$$+ x^3 L^2 \left(3c_3 - 2b_2\beta_0 - 5b_2\gamma_0 \right) + \mathcal{O}(x^4). \tag{10}$$

For $n_f = 5$ we see from (6) that the coefficients of x, x^2, and $x^2 L$ vanish, as required. The requirement that $O(x^3)$ coefficients in (10) also vanish may be used to determine the logarithmic coefficients c_1, c_2, and c_3 within $S[x, L]$. For $n_f = 5$, we find from (6) and (10) that

$$c_1 = 249.592, \quad c_2 = 178.755, \quad c_3 = 50.9144. \tag{11}$$

The coefficient c_0, however, is RG-inaccessible to the order we are working, and must be obtained via a direct three-loop calculation.

PADÉ-APPROXIMANT ESTIMATION OF NEXT-ORDER TERMS

In the absence of a direct calculation, Padé-approximant methods provide a means for estimating next-order terms in a perturbative series, provided such a series obeys appropriate criteria generally believed to be applicable to field-theoretical perturbative series [4]. As an example of the power of such methods, consider the following perturbative series:

$$S = 1 - x + \frac{1}{2}x^2 - \frac{1}{3}x^3 + \frac{5}{24}x^4 + \ldots . \tag{12}$$

This series is, in fact, the first five terms of the Maclaurin expansion of the function $S(x) = \sec(x) - \tan(x)$. A $[N|M]$ Padé approximant to a series is the ratio of degree-N and degree-M polynomials that replicates the known terms of a series. For example, the $[2|2]$ approximant which replicates the series (12) is specified (up to a common scale factor for the numerator and denominator) by

$$S^{[2|2]} = \frac{1 - \frac{x}{2} - \frac{x^2}{12}}{1 + \frac{x}{2} - \frac{x^2}{12}}. \tag{13}$$

Specifically, the Maclaurin expansion of $S^{[2|2]}$ is

$$S^{[2|2]} = 1 - x + \frac{1}{2}x^2 - \frac{1}{3}x^3 + \frac{5}{24}x^4 - \frac{19}{144}x^5 + \dots . \tag{14}$$

The final series term in (14) may be regarded to be a Padé-approximant prediction for the next term in the series (12). This prediction is surprisingly accurate, as the underlying function's Maclaurin series expansion is

$$\sec(x) - \tan(x) = 1 - x + \frac{1}{2}x^2 - \frac{1}{3}x^3 + \frac{5}{24}x^4 - \frac{2}{15}x^5 + \dots . \tag{15}$$

We see that the final series terms listed in (14) and (15) are quite close: $19/144 (= 0.13194 \dots) \cong 2/15 (= 0.13333 \dots)$.

In the calculation of the $B \rightarrow X_u \ell^- \overline{\nu}_\ell$ decay rate, the particular series with which we are concerned is of the form

$$S[x, L] = 1 + R_1[L]x + R_2[L]x^2 + R_3[L]x^3 + \dots , \tag{16}$$

with

$$R_1[L] = a_0 + a_1 L, \quad R_2[L] = b_0 + b_1 L + b_2 L^2 \tag{17}$$

fully determined by the previously-calculated coefficients (6), and with the next order coefficient

$$R_3[L] = c_0 + c_1 L + c_2 L^2 + c_3 L^3 \tag{18}$$

assumed to be unknown. Of course, c_1, c_2, and c_3 are in fact accessible by RG methods [they are listed in (11)]; we will ultimately compare Padé-estimates to RG-determinations of these coefficients to ascertain the accuracy of the Padé-estimation procedure we utilise to obtain the RG-inaccessible constant c_0.

We seek a procedure to estimate R_3 in terms of the known lower order coefficients R_1 and R_2 appearing in (16). To do this, we assume that the error of an $[N-1|1]$ approximant in estimating the $N+1^{th}$ term in a series is inversely proportional to N. For example, the $[0|1]$ approximant to the series $1 + R_1 x + R_2 x^2 + R_3 x^3 + \dots$ is just

$$S^{[0|1]} = \frac{1}{1 - R_1 x} = 1 + R_1 x + R_1^2 x^2 + \dots . \tag{19}$$

The predicted coefficient of x^2 in (19) is $R_2^{[0|1]} \equiv R_1^2$, as opposed to the true coefficient R_2. We find the relative error of the $[0|1]$ approximant in predicting R_2 to be

$$\delta_{[0|1]} \equiv \frac{R_2^{[0|1]} - R_2}{R_2} = \frac{R_1^2 - R_2}{R_2}. \tag{20}$$

Similarly the $[1|1]$ approximant to the same series is

$$S^{[1|1]} = \frac{1 + (R_1 - R_2/R_1)x}{1 - (R_2/R_1)x} = 1 + R_1 x + R_2 x^2 + \left(R_2^2/R_1\right)x^3 + \dots . \tag{21}$$

The predicted coefficient of x^3 is R_2^2/R_1, which we denote as $R_3^{[1|1]}$, and the relative error associated with this prediction is

$$\delta_{[1|1]} \equiv \frac{R_3^{[1|1]} - R_3}{R_3} = \frac{R_2^2/R_1 - R_3}{R_3}. \tag{22}$$

If the relative error of an $[N-1|1]$ approximant in predicting R_{N+1} is inversely proportional to N, i.e., if

$$\delta_{[N-1|1]} \equiv \frac{R_{N+1}^{[N-1|1]} - R_{N+1}}{R_{N+1}} = -\frac{A}{N}, \tag{23}$$

as suggested in [5], we see from (20) and (23) that $A = 1 - R_1^2/R_2$. Since (23) also implies that $\delta_{[1|1]} = -A/2$, we can use (22) to obtain an error-improved estimate of R_3 entirely in terms of the known series terms R_1 and R_2 [6]:

$$R_3 = 2R_2^3/[R_1^3 + R_1 R_2]. \tag{24}$$

ESTIMATION OF THREE-LOOP COEFFICIENTS

The problem with the prediction (24) for the calculation considered here is the incompatibility of R_3 as a degree-3 polynomial in L (18) with the rational (non-polynomial) function of L one obtains via substitution of (17) into (24). One approach to this problem is to generate a least squares fit of (24) to the form (18) over the perturbative portion of the domain of $L(\mu)$, i.e., over the ultraviolet domain $\mu > m_b(\mu)$. We define $w \equiv m_b^2(\mu)/\mu^2$, in which case $L = -\log(w)$ from (4), and obtain a least squares fit of (18) to (24) over the range $0 \leq w \leq 1$ [i.e., $\mu \geq m_b(\mu)$] by optimizing the function [7]

$$\chi^2(c_0, c_1, c_2, c_3)$$

$$\equiv \int_0^1 dw \left[\frac{2R_2^3(w)}{R_1^3(w) + R_1(w)R_2(w)} - \left(c_0 - c_1 \log(w) + c_2 \log^2(w) - c_3 \log^3(w) \right) \right]^2 \tag{25}$$

with respect to c_i, the polynomial coefficients of powers of L within (18). Upon substitution of the known [via (6) and (17)] functions $R_1(w) = a_0 - a_1 \log(w)$, $R_2(w) = b_0 - b_1 \log(w) + b_2 log^2(w)$ into the integrand of (25), we find from explicit numerical integration that

$$\chi^2(c_0, c_1, c_2, c_3) = c_0^2 + 2c_1^2 + 24c_2^2 + 720c_3^2 + 2c_0 c_1 + 4c_0 c_2 + 12c_0 c_3$$

$$+12c_1 c_2 + 48c_1 c_3 + 240c_2 c_3 - 2237.27c_0 - 5980.96c_1$$

$$- 24423.1c_2 - 129077c_3 + 6386542. \tag{26}$$

The four conditions $\partial\chi^2/\partial c_i = 0$ ($i = \{0, 1, 2, 3\}$) provide the following Padé-estimates for c_i:

$$c_0 = 198, \ c_1 = 261, \ c_2 = 184, \ c_3 = 48.6 \ . \tag{27}$$

Note the excellent agreement of estimates for $\{c_1, c_2, c_3\}$ with the true values (11) obtained via RG methods. The relative errors $\delta c_i \equiv (c_i - c_i^{RG})/c_i^{RG}$ in the Padé estimates are respectively $\delta c_1 = -4.6\%$, $\delta c_2 = 2.9\%$, $\delta c_3 = 2.1\%$. These small errors suggest similar accuracy in the determination of the unknown coefficient c_0. Utilizing this value of c_0 in the $L = 0$ limit, appropriate for the $\mu = m_b(\mu)$ choice of renormalization scale in (1), we find that the series within (1) is now improved to

$$\Gamma\left(B \to X_u \ell^- \overline{\nu}_\ell\right) = K(4.17\, GeV)^5 [1 + 0.304 + 0.137 + 0.075] = K(1913\, GeV^5). \tag{28}$$

The estimate (28) is obtained using the central value of Chetyrkin and Stein-hauser's [8] determination of $m_b(m_b) = 4.17 \pm 0.05\, GeV$ an estimate which followed from a central value $\alpha_s(M_z) = 0.118$ [also utilized to evolve $x(\mu)$ in (28)].

RESIDUAL SCALE DEPENDENCE

The series within the rate (28) is evaluated at $\mu = 4.17\, GeV$ and appears to be the first four terms of a positive-term perturbative series. This positive-term character is evident for $\mu > 4.17\, GeV$ as well, the domain of $L(\mu)$ for which L is positive, since the coefficients a_i, b_i, and c_i (including the estimated value for c_0) are all positive. If convergent, a truncated positive-term series necessarily underestimates the series sum. For values of μ larger than $4.17\, GeV$, this underestimation is even more severe, because of the positive growth of $L(\mu)$. Thus $\Gamma(\mu = 9\, GeV) = K(1733\, GeV^5) < \Gamma(\mu = 4.17\, GeV)$, as evident from (28).

As noted in [1], the perturbative series does not become locally flat until μ is well into the infrared region. This region [$\mu < m_b(m_b)$] can be accessed via threshold matching conditions [9] to a running coupling constant and running mass characterized by four active flavours:

$$x^{(4)}\left[m_b(m_b)\right]$$

$$= x^{(5)}\left[m_b(m_b)\right]\left[1 + 0.1528\left(x^{(5)}\left[m_b(m_b)\right]\right)^2 + 0.633\left(x^{(5)}\left[m_b(m_b)\right]\right)^3\right], \tag{29}$$

$$m_b^{(4)}\left[m_b(m_b)\right]$$

$$= m_b^{(5)}\left[m_b(m_b)\right]\left[1 + 0.2060\left(x^{(5)}\left[m_b(m_b)\right]\right)^2 + 1.95\left(x^{(5)}\left[m_b(m_b)\right]\right)^3\right]. \tag{30}$$

If $\alpha_s(M_z) = 0.118$ and $m_b^{(5)}(m_b) = 4.170\,GeV$, the conditions (29) and (30) imply that $x^{(5)}(4.170\,GeV) = 0.07155$, $x^{(4)}(4.170\,GeV) = 0.07162$, and $m_b^{(4)}(4.170\,GeV) = 4.177\,GeV$. Moreover, with 4 active flavours the two-loop constants characterising the rate (5) are no longer as given in (6); instead one finds for $n_f = 4$ that [1]

$$b_0 = 25.7547, \ b_1 = 38.3935, \ b_2 = 17.7083, \tag{31}$$

and, from perturbative RG-invariance (10) with constants β_i and γ_i characterized by four active flavours,

$$c_1 = 263.84, \ c_2 = 194.23, \ c_3 = 54.109. \tag{32}$$

One can also obtain estimates of the $n_f = 4$ three-loop coefficients via optimization of the χ^2 function (25):

$$c_0 = 181.5, \ c_1 = 277.3, \ c_2 = 197.6, \ c_3 = 51.86. \tag{33}$$

The startlingly close agreement between (32) and (33) for the RG- accessible coefficients c_1, c_2, c_3 is indicative of comparable accuracy for the estimate of c_0 in (33).

In ref. [10], it is shown that the $n_f = 4$ values for c_i are consistent with continuity of the rate $\Gamma(B \to X_u \ell^- \overline{\nu}_\ell)$ across the $n_f = 5$ threshold at $4.17\,GeV$. The rate is shown to increase with decreasing μ until a local maximum is reached at $\mu = 1.775\,GeV$ [10]:

$$\left(\frac{d\Gamma}{d\mu} |_{\mu=1.775\,GeV} \right) = 0, \tag{34}$$

$$\Gamma\left[\mu = 1775\,GeV\right]$$

$$= K\left[m_b^{(4)}(1.775\,GeV)\right]^5 [1 - 0.6455 + 0.2477 - 0.0143] = K(2071\,GeV^5). \tag{35}$$

The optimisation condition (34) ensures that $\mu = 1.775\,GeV$ is the choice of μ for which there is minimal residual scale sensitivity of the rate, an established criterion for the choice of scale [3]. Note that the perturbative series within (35) is now an *alternating series* whose 3-loop term is much smaller than that in (28). The alternation of sign becomes possible because $L(\mu)$ is negative when $\mu < m_b(\mu)$, as evident from (4). If the series within (35) continues to be both alternating and montonically decreasing, the rate at $\mu = 1.775\,GeV$ can be shown to be bounded from below *and* above:

$$K \times 2071\,GeV^5 \le \Gamma\left[\mu = 1.775\,GeV\right] \le K \times 2122\,GeV^5. \tag{36}$$

Remarkably, the "minimal-sensitivity" point defined by (34) is quite close to the point at which the three-loop term vanishes entirely, a point at which three-loop estimation of the series, if asymptotic, would be most accurate. With RG-values

(32) for c_1, c_2, c_3 and the Padé- estimate $c_0 = 188.5$ for c_0 [corresponding to minimization of χ^2 with respect to c_0 after explicit incorporation of RG-values of c_1, c_2, c_3 into (25)], the three loop term (18) is seen to *vanish* at $\mu = 1.835\,GeV$, at which point $\Gamma(\mu = 1.835\,GeV) = K \times 2069\,GeV^5$. The agreement between this value for the rate with the minimal-sensitivity estimate (35) is striking.

$|V_{ub}|$: THEORETICAL UNCERTAINTIES

The minimal sensitivity rate (35) is subject to the following $\Delta\Gamma/K$ theoretical uncertainties: truncation error (t.e.)

$$|\Delta\Gamma/K|_{\text{t.e.}} = \left[m_b^{(4)}(1.775)\right]^5 (0.0143) = 51\,GeV^5, \tag{37}$$

error in estimating c_0 $\left(|\Delta c_0/c_0| \simeq |\Delta c_i/c_i^{RG}| \simeq 5\%\right)$,

$$|\Delta\Gamma/K|_{c_0} = 35\,GeV^5, \tag{38}$$

uncertainty in $\alpha_s(M_z)(= 0.119 \pm 0.002\ [2])$,

$$\Delta\Gamma/K|_{\alpha_s} = \left(\begin{array}{c} +108 \\ -28 \end{array}\right) GeV^5 \tag{39}$$

(asymmetric bounds are because (35) is based upon $\alpha_s(M_z) = 0.118$), uncertainty in $m_b(m_b)(= 4.17 \pm 0.05\ [8])$,

$$\Delta\Gamma/K|_{m_b} = \left(\begin{array}{c} +120 \\ -115 \end{array}\right) GeV^5, \tag{40}$$

and the asymmetric nonperturbative (n.p) contribution to the overall rate [11]:

$$\Delta\Gamma/K|_{\text{n.p.}} = \left(\begin{array}{c} -39 \\ -57 \end{array}\right) GeV^5. \tag{41}$$

Inclusive of all these contributions, the result (35) becomes

$$\Gamma = K \times (2065 \pm 14\%)GeV^5. \tag{42}$$

Using (1) for the coefficient K, the branching ratio for inclusive charmless semileptonic decay is seen to be

$$R \equiv \Gamma\left(B \to X_u \ell^- \overline{\nu}_\ell\right)/\Gamma(B \to \text{anything}) = \frac{|V_{ub}|^2 G_F^2}{192\pi^3}\frac{[(2065 \pm 14\%)GeV^5]}{4.25 \cdot 10^{-13}GeV}, \tag{43}$$

in which case

$$|V_{ub}| = (0.0949 \pm 0.0066)R^{1/2}. \tag{44}$$

The central value of (44) is in agreement with Uraltsev's relation between $|V_{ub}|$ and the branching ratio [12], and is indicative of an overall $\pm7\%$ theoretical uncertainty in this relation.

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